Complex Rheology in a Small Lattice Gas System

Awazu, Akinori

Complex Rheology in a Small Lattice Gas System

Akinori Awazu
Department of Physics, University of Tokyo,
Hongou 7-3-1, Bunkyou-ku, Tokyo 113-0033, Japan.

要旨:ある簡単な少数自由度格子ガスモデルで実現された、(高分子、コロイド溶液系等でよく見られる) Shear-Thinning、Shear-Thickening とよく似た現象について紹介する。

Introduction - The transport phenomena of a nonequilibrium lattice gas system are investigated. Here, nonequilibrium lattice gases are simple mathematical models, which have been useful and important in studies of the several properties of nonequilibrium systems with numerous degrees of freedom. In this paper, we focus on a lattice gas system with a periodic boundary, which consists of only two particles interacting repulsively and the potential forces acting on them.

In such a simple system, the following complex transport properties are found when only one particle is driven by an external driving field; With the increase in the mean velocity of the driven particle, the coefficient of effective drag of this particle (=[driving field strength]/[mean velocity]) varies in the form, increase → decrease → increase → decrease under certain conditions. Moreover, under other conditions, the relation between these values show changes similar to those between shear rate and shear viscosity observed experimentally in the shear-thickening polymer[1] or colloidal suspensions[2]; With the increase in the mean velocity, the coefficient of effective drag varies in the form, increase → decrease or decrease → increase → decrease.

Model - We consider a lattice system with two parallel one-dimensional lanes where each lane involves L sites with a periodic boundary. Each lane contains only one particle which

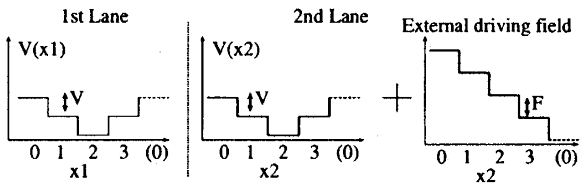

Figure 1: Illustrations of effects of potential and external field in each lane.

moves randomly to the nearest sites without changing lanes. The sites occupied by particles in the 1st and 2nd lanes are denoted x_1 and x_2, respectively, which are given as integer numbers from 0 to $L-1$.

The effect of potential forces acting on the particles is described by the following Hamiltonian: $H(x_1, x_2) = V(x_1) + V(x_2) + V_{12}(x_1, x_2)$, where $V(x)$ represents the one-body potential on each lane, and $V_{12}(x_1, x_2)$ represents the interaction potential between the two particles. Furthermore, an external driving field is applied to the particle on the 2nd lane. We denote the field strength F.

The time evolution of this system is described by the iteration of the following three steps. First, one of the two particles is randomly chosen. Let the position of the chosen particle be x. Second, its neighboring site y, $x-1$ or $x+1$, is randomly chosen. Third, the chosen particle moves from x to y with the following probability $c(x, y; x_1, x_2) = \frac{1}{1+\exp[Q(x \to y; x_1, x_2)/T]}$, with $Q(x \to y; x_1, x_2) = H(x'_1, x'_2) - H(x_1, x_2) - F(x'_2 - x_2)$, where $(x'_1, x'_2) = (x_1, y)$ when $x = x_2$, and $(x'_1, x'_2) =$

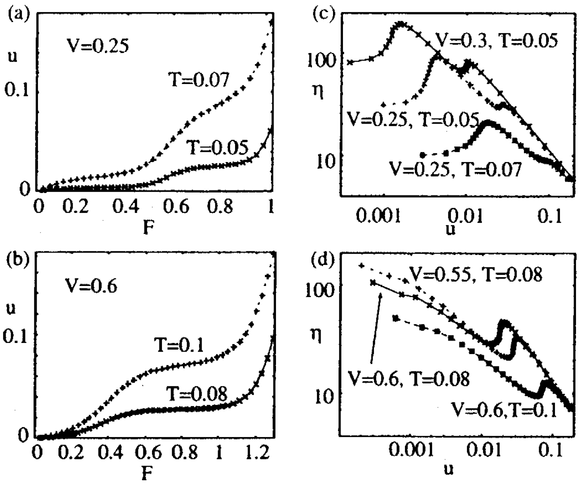

Figure 2: (a)(b) u as a function of F, and (c)(d) η as a function of u.

(y, x_2) when $x = x_1$. Here, T is temperature, and the time step is given by [No. of above iterations]/[No. of particles $(= 2)$].

Specifically, we study the case where $L = 4$, $V(x) = V|L/2 - x|$ (Fig. 1), and $V_{12}(x_1, x_2) = I\delta_{x_1,x_2}$ using the $L \times L$ unit matrix δ_{ij}.

Results and discussions - Now, we show the simulation results of this system. We mainly focus on the cases with $V < I$ and $|F| < I+V$, and T is small enough compared to I and V. In order to characterize the system, we define the mean velocity of the driven particle (in the 2nd lane) in steady state, u, as the difference of the long time average of the moving ratio of the driven particle in the positive and negative directions. Here, the direction $x_i : 0 \to 1 \to \ldots \to (L-1) \to 0 \to$ is positive. For simplicity, $I = 1$ and $F > 0$ are set.

Figures 2(a) and (b) show u as a function of F for (a) $V = 0.25$ with $T = 0.05$ or $T = 0.07$ and (b) $V = 0.6$ with $T = 0.08$ or $T = 0.1$. As shown in them, two types of $F-u$ relations, i) u increases steeply with F, ii) u increases slowly with F, appear depending on the range of F. From these results, the relations between u and the coefficient of effective drag of the driven particle η defined as F/u are straightforwardly obtained. Figures 2(c) and (d) show η as a function of u for (c) $V = 0.25$ or $V = 0.3$ with $T = 0.05$ or $T = 0.07$ and (d) $V = 0.55$ or $V = 0.6$ with $T = 0.08$ or $T = 0.1$. As shown in Fig. 2(c), η varies in the form, increase $\to$ decrease $\to$ increase $\to$ decrease, with the increase in u in the case with $V < I/2$ and a small T (for example $V = 0.3$ and $T = 0.05$).

When the smaller V and a little larger T are given (for example, $V = 0.25$ and $T = 0.07$), the change in η becomes less sharp, and simpler in the form, increase $\to$ decrease, with the increase in u (Fig. 2(c)). In this case, the $u-\eta$ profile is given in a form qualitatively similar to that between the shear rate and shear viscosity coefficient of the shear-thickening polymer solutions obtained experimentally[1].

On the other hand, if a larger V is given as in the range $I/2 < V < I$ (for example, $V = 0.55$ and $V = 0.6$), η varies in the form, decrease $\to$ increase $\to$ decrease, with the increase in u independently of T (Fig. 2(d)). In this case, the $u-\eta$ profile appears qualitatively similar to that between the shear rate and shear viscosity coefficient of the shear-thickening colloidal solutions obtained experimentally[2]. (If T is given larger, $u-\eta$ profiles for several V become less sharp and close to flat like Newtonian fluid continuously.)

These results can be easily explained by the considerations of the transition probabilities among (x_1, x_2) ((x_1, x_2): $(0,0) \sim (3,3)$.)[3]. We expect our results to provide important hints to uncover the possible mechanism for several rheological characteristics of several soft materials.

References

[1] S X. Ma and S L. Cooper, Macromolecules **34** (2001) 3294.

[2] E. Bertrand, J. Bibette and V. Schmitt, Phys. Rev. E **66** (2003) 060401.

[3] A. Awazu, To appear in Physica A.